

# Time Dependent Current Oscillations Through a Quantum Dot

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## I. ABSTRACT

Time dependent phenomena associated to charge transport along a quantum dot in the charge quantization regime is studied. Superimposed to the Coulomb blockade behaviour the current has novel non-linear properties. Together with static multistabilities in the negative resistance region of the I-V characteristic curve, strong correlations at the dot give rise to self-sustained current and charge oscillations. Their properties depend upon the parameters of the quantum dot and the external applied voltages.

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## II. INTRODUCTION

Electron correlation effects on the transport properties of a quantum dot (**QD**) under the influence of an external potential have been the subject of many experimental and theoretical studies in recent years. This device although possesses thousands of atoms behaves as if it were an artificial atom due to its discrete energy spectrum. The enormous advantages of this artificial atom are that its properties can be modified continuously by adjusting the external potentials applied to it [1]. Unlike a real atom it can be experimentally isolated and its transport properties obtained studying the flow of charges through it. The quantization of charge and energy plays the major role in the transport properties of a **QD**. The conductance exhibits oscillations as a function of the external potential which can be explained in terms of a transport mechanism governed by single-electron tunneling and Coulomb blockade effect due to the e-e interaction inside the dot[2].

It is well established that the Coulomb interaction produces non-linear effects in **3D** double barrier heterostructure, observed as intrinsic static bistability in the negative differential resistance region of the I-V characteristic curve of the device[3]. This property has been explained as an electrostatic effect due to the e-e interaction among the charges inside the well. Besides this static behavior, theoretical studies have proposed that the Coulomb interaction can produce time dependent oscillations[4]. More recently current oscillations promoted by an external magnetic field applied in the direction of the current were predicted[5]. These last results showed that the system bifurcates as the field is increased and may transit to chaos at large enough fields. Recently very interesting experimental evidences of the existence of these oscillations induced by an external magnetic field, have been given[6].

Although Coulomb interaction phenomena have been a matter of great concern in the last years, to the best of our knowledge, there have not been experimental studies reporting neither static bistabilities nor current and charge oscillations through a **QD**. In the search for stationary behavior, we were able to theoretically predict a bistability similar to the one that appears in the I-V characteristic curve of a **3D** double barrier heterostructure. We obtained as well evidences of the non-existance of stationary solutions in some regions of the parameter space for the currents flowing through the **QD**[7].

In this communication letter we address the study of currents going through a **QD** connected to leads under the effect of an external potential. We report the existence of static hysteresis behavior of the current in the negative resistance region. What is more important, we find novel time dependent phenomena which appear as self-sustained current and charge oscillations with properties depending on the internal parameters of the system and the external applied potentials. These time dependent phenomena are derived from the highly correlated electrons inside the **QD**.

It has been shown that the physics associated to a **QD** connected to two leads can be readily understood in terms of a single magnetic impurity Anderson Hamiltonian, where the impurity is the quantum dot[2]. The leads can be represented by a **1D** tight-binding Hamiltonian connecting the dot to particle reservoirs characterized by Fermi levels  $E_l$  and  $E_r$ . The difference  $E_l - E_r$  gives the bias voltage applied to the system when connected to a battery. The Hamiltonian is given by

$$H = \sum_{i\sigma} \epsilon_i n_{i\sigma} + v \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + (\epsilon_o + V_g) \sum_{\sigma} n_{o\sigma} + U n_{o\uparrow} n_{o\downarrow}. \quad (1)$$

The diagonal matrix element  $\epsilon_i$  is site dependent because it takes into account the potential profile and the two barriers. The gate voltage  $V_g$  is supposed to be effective only on the **QD**. Since we are not interested in very low temperature physics, as for instance the Kondo effect, we use a decoupling procedure[8] to solve the equation of motion for the one particle operator. Although this is a simple approximation, it is adequate to treat high correlations at the dot, responsible for Coulomb blockade phenomena[2]. The non-linear behavior stems from the dependence of the solution upon the self-consistent calculated charge content of the dot. As we are not interested in studying magnetic properties, we omit the subindex  $\sigma$  corresponding to the spin. Using the set of Wannier functions localized at site  $i$ ,  $\phi_i(r)$ , we can write the time dependent state  $\varphi_k(r, t)$  as,

$$\varphi_k(r, t) = \sum_i a_i^k(t) \phi_i(r) \quad (2)$$

The probability amplitude for an electron to be at site  $j$  in a time dependent state  $\varphi_k(r, t)$  is given by the equation of motion,

$$i\hbar \frac{da_j^k}{dt} = \epsilon_j a_j^k + v(a_{j-1}^k + a_{j+1}^k) \quad (i \neq 0) \quad (3)$$

$$i\hbar \frac{da_o^{k,\alpha}}{dt} = (\epsilon_o^\alpha + V_g) a_o^{k,\alpha} + n^\alpha v(a_{-1}^k + a_1^k) \quad (4)$$

where  $\alpha = \pm$ ;  $n^+ = n$ ;  $n^- = 1 - n$ ;  $\epsilon_o^+ = U$ ;  $\epsilon_o^- = 0$  and  $n$  is the number of electrons per spin at the dot that is calculated from the probability amplitudes by the equation,

$$n = 2 \int_0^{k_f} |a_o^k|^2 dk \quad (5)$$

where  $a_o^k = a_o^{k,+} + a_o^{k,-}$  and  $k_f$  is the Fermi wave vector of the emitter side. We have assumed for simplicity that the collector is not doped so that the charge that goes towards the emitter is restricted to the electrons that have been reflected on the barriers. The time dependent equations are solved by discretizing equations (3) and (4), and using a half-implicit numerical method, which is second-order accurate and unitary[9].

The solution of these equations require the knowledge of the wave function at  $-\infty$  and  $+\infty$ . We suppose that an incident electron of wave vector  $k$  is described by the function,

$$a_j^k = (I e^{ikx_j} + R_j e^{-ikx_j}) e^{-i\epsilon t/\hbar} \quad (x_j \leq -L) \quad (6)$$

$$a_j^k = T_j e^{ik'x_j} e^{-i\epsilon t/\hbar} \quad (x_j \geq L) \quad (7)$$

where the system is explicitly defined between  $-L$  and  $L$  and  $k'$  is the wave vector of the transmitted particle  $k' = \sqrt{\left(\frac{2m(E_l - E_r)}{\hbar^2}\right) + k^2}$ . The incident amplitude  $I$  is assumed to be spatially constant. Instead, far from the barriers, the envelope function of the reflected and transmitted waves  $R_j$  and  $T_j$  are supposed to be weakly dependent on site  $j$ . This permits to restrict the dependence to the linear term, which results to be an adequate approximation provided the time step taken to discretize equations (3) and (4) is less than certain limit value that depends upon the parametrization of the system. A maximum value of  $0,3fs$  was adequate to guarantee numerical stability up to 200 ps. To eliminate spurious reflections at the boundary it was necessary to take systems of the order of  $2L = 400$  sites. In the numerical procedure, the Wannier intensities obtained for one bias are used as the starting point for the next bias step. Once the Wannier intensities are known the current is calculated from[9],

$$J_j \propto 2 \int_o^{k_f} \left[ \text{Im}(a_j^{k*} (a_{j+1}^k - a_j^k)) \right] dk \quad (8)$$

It is important to emphasize that the system we study has to be in the Coulomb blockade regime. Charge quantization is obtained satisfying the relation  $\frac{t'^2}{W} < U$  where  $t'$  is an effective coupling constant between the **QD** and the leads controlled by the barriers parameters and  $W$  is the leads bandwidth. In this case the energy spacing  $U$  between the states with  $N$  and  $N + 1$  electrons is greater than the width of the resonant levels within the dot.

We study the system defined by an emitter barrier of  $1.4eV$  and a collector barrier of  $2.4eV$  both of a thickness of 5 lattice parameters and an electronic repulsion  $U = 20\text{meV}$ . This configuration represents a GaAs structure in

the charge quantization regime. A similar effective coupling constant can be obtained assuming lower and thicker barriers. We have chosen the case with less number of sites in order to reduce the computational effort. In order to enhance the charge content of the dot and consequently the non-linear effects the second barrier is taken to be higher than the first. The Fermi level lies 30 meV above the bottom of the emitter conduction band. With these parameters and zero gate voltage and bias the localized level at the dot lies well above the Fermi level, so that the system is completely out of resonance. For small values of the gate potential equations (3) and (4) have a stationary solution after a transient, for the whole interval of bias voltage  $V$ , which drives the system into and off resonance. Increasing the gate potential the system enters into a completely different regime. As the bias voltage required to drive the system into resonance is small, because the resonant level is now near the Fermi level, the second barrier is not significantly reduced by the bias voltage and is able to trap a large amount of electronic charge inside the dot. As a consequence, the non-linear effect is enhanced giving rise to a region in the I-V characteristic curve where there is no stationary solution. In this parameter region the current has self-sustained oscillations while for greater values of the bias voltage the system possesses complex electrostatic multistabilities which can be obtained, depending upon the initial condition, augmenting or diminishing the bias voltage. These static multistabilities are very well known phenomena of **3D** systems, although they generally assume a bistable structure[3]. The situation for the **QD** described is illustrated in Fig. 1 where the bubble shows the maximum and minimum of the current oscillations, while for a greater value of the bias voltage the electrostatic instabilities are clearly represented. The non-stationary solutions lie outside the static multistable region for small values of  $V_g$ . However, for larger values of  $V_g$ , there is a superposition of the regions where both effects are active. The static large multistability is related to the drop of the resonant level below the bottom of the conduction band, while the dynamic oscillations appear when the resonant level aligns with the Fermi level. The size and location of the oscillating behavior in the I-V space depends upon the gate voltage. Its size increases with  $V_g$ . The non-linearities are enhanced by the gate potential, constituting an external tunable parameter through which the oscillating phenomena can be controlled.

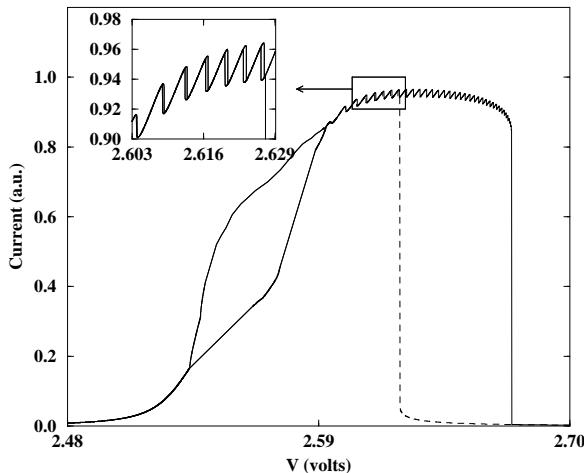


FIG. 1. Current versus bias voltage, I-V characteristic curve. The bubble indicates the maximum and minimum of the oscillating current amplitude. The inset shows a complex structure of static bistable behaviour. Dashed line shows the uncharged **QD** solution.

We have taken different values of the bias  $V_g$  to study explicitly the time dependent current going along the device. For  $V_g = 0.2$  volts the system possesses a stationary solution for all values of the bias voltage. For a greater value of the gate potential  $V_g = 0.86$  volts and  $V = 5.6$  volts, we show the current and the charge as a function of time in three different locations of the system: in the emitter and collector side before and after the barriers, in Fig. 2b and, inside the dot, in Fig. 2c. We see that after a transient of some ps, the system begins to oscillate in a self-sustained way. It is important to note the different behaviors of the oscillations depending upon the site where the current is evaluated. The oscillations are large in the region before the emitter barrier and inside the well, while after the charge has passed through the device the more opaque collector barrier damps the oscillation in a very significant way. Although not perfectly periodic, the oscillations have some regularity. The frequency spectrum is continuous with the predominance of two and some times three well define frequency regions. The origin of this behavior is not completely clear to us. However, the existence of more than one frequency region has to be attributed to the amount of non-linearity in the system. A less non-linear situation, obtained for instance in the near vicinity of the bifurcation point where time dependent behavior appears in the I-V characteristic curve of Fig. 1, shows small amplitude oscillating currents of almost only one frequency. Very remarkably, superimposed to the oscillating currents, we exhibit in the inset of Fig.

2c very high frequency oscillations greatly enhanced inside the well and almost non-existent outside it. We attribute them to the electrons going back and forth inside the well with a period corresponding to the time taken by the electrons at the neighborhood of the Fermi energy being successively reflected by the barriers.

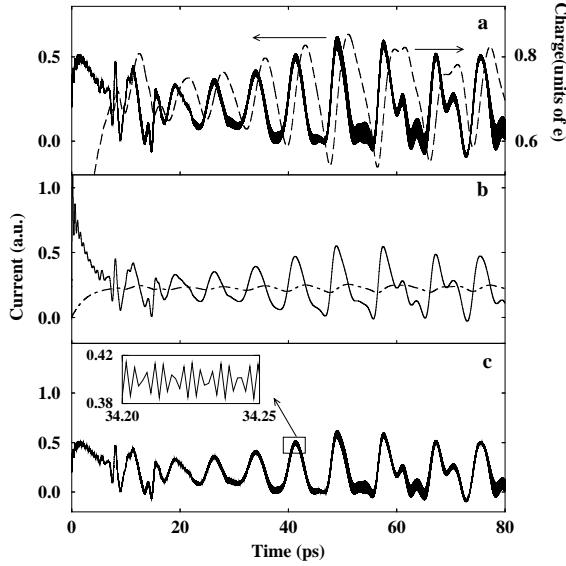


FIG. 2. Current and charge versus time for  $V_g = 0.86$  volts and  $V = 5.6$  volts. a) Charge (dashed line) and current (full line) at the dot as a function of time, showing the time lag between them. b) Current at the emitter (full line) and at the collector (dashed line). c) Current at the dot. Inset shows high frequency oscillations.

Changing the gate potential the dot enters into resonance when its local level aligns with the Fermi level. The current increases abruptly and, due to the trapping effect of the collector barrier, the dot charge per spin  $n$  assumes its maximum value after a time. As a consequence, the strength of the resonant level, which due to many body effects depends upon the dot charge as  $(1 - n)$ , diminishes and the flow of electrons going into the dot reduces. As time evolves, the total amount of charge inside the dot drops because the leaking of charge through the second barrier becomes greater than its entrance through the first one. The reduction of charge increases the strength of the resonant level, which increases the flowing current starting a new cycle. As we have numerically verified, for a configuration outside the Coulomb blockade regime, by diminishing for instance the first barrier, the oscillations are damped out and the system reaches a stationary regime. In this case, as the system is driven into resonance, the current increases and the dot charge reacts almost instantaneously with no significant lag time between them.

To generate self-sustained current oscillations the system has to be in a parameter region where there is no dynamic accommodation between the current and the charge inside the dot. It requires an abrupt entrance in resonance when the external potential is modified. This is the case of the charge quantization regime when the channel for the electron to go through is provided by the very sharp resonant peak inside the dot. It is interesting to compare the current and the charge oscillations inside the well in this case. Although the frequencies and the general properties of both oscillating quantities are the same, there is a clear lag time  $\tau$  of the dot charge in relation to the current. The dephasing between charge and current which disappears with more transparent barriers is illustrated in Fig. 2a. It is clear that the lag  $\tau$  depends upon the time scale controlling the entrance of the charge into the resonant state, which is called the buildup time. For opaque emitter barriers, as in our case, the buildup time is found to be essentially independent of the barrier parameters. The buildup process is essentially determined by the spatial distribution of the extra charge in conditions to enter into the well[10]. This is slightly different in each oscillation, creating a rather irregular lag among the two quantities as time goes along, as exhibited in Fig. 2a.

Due to computer time limitations it was not possible to develop a systematic investigation of the phenomenon. However, we have studied the system modifying some of its parameters in order to give support to the interpretation above. There is a clear tendency of the oscillation mean value frequency to increase reducing the opacity of the barriers although it is more clearly dependent upon the second barrier. This is consistent with the interpretation given above as it is the collector barrier that controls the leaking time of the charge when its entrance is abruptly reduced by non-linearity. In order to study the stability of the self-sustained oscillations we have calculated, for one particular case, the time evolution of the system up to a value of 200ps. The oscillations maintain their amplitude and regular shape. We have taken a charged and a discharged dot as two different initial conditions. The first condition creates oscillations immediately after the circuit is switched on while in the second the system goes through a transient during

which the dot is charged, as shown in Fig. 3. Although the oscillations have a similar behavior shifting one relative to the other by this charging time, there are differences which in fact increase in time as shown in the inset of Fig. 3. In certain regions of the parameter space the oscillations result to be very sensitive to initial conditions, suggesting the existence of chaotic phenomena.

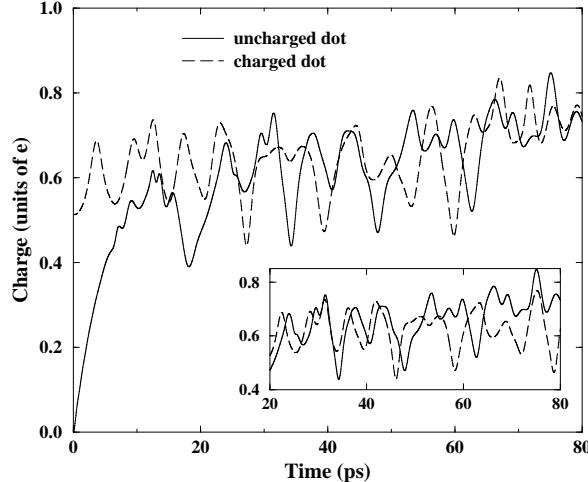


FIG. 3. Charge at the dot as a function of time,  $V = 3.13$  volts and  $V_g = 3.02$  volts. Initial states, dot uncharged (full line) and dot charged (dashed line). Inset shows the two solutions where the dot uncharged initial state solution is shifted by the changing time.

We have done a time dependent study of the current circulating through a QD in the Coulomb blockade regime. We conclude that together with complex static multistable behavior, non linearity produced by highly correlated electrons in the dot give rise to charge and current time dependent oscillations. They can be controlled by changing the parameters defining the system and the various external potentials applied. A complete characterization of the time dependent oscillations would require a great computational effort, which could be justified only in the case of an experimental verification of the phenomena theoretically predicted in this letter.

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